GreenScreen[®] Assessment for [*N-alkoxy Hindered Amine Reaction Products (CAS#191680-81-<u>6)</u>]*

Method Version: GreenScreen[®] Version 1.2¹

Verified or Non-Verified²: <u>NON-VERIFIED</u>

Introduction^{3,4,5}

This GreenScreen assessment is based on the information reported in the corresponding chemical hazard profile in "An Alternatives Assessment for the Flame Retardant Decabromodiphenylether (DecaBDE) Final Report"³. Additional information on hazard endpoints beyond what was included in the final report was not sought with the exception of reactivity. Hazard classification information for reactivity was supplemented because it is not included in the DfE report but is needed to apply the GreenScreen Benchmark system.

Hazard classification levels reported in the DfE profiles and in this GreenScreen report may differ due to differences between criteria as defined in the DFE "Alternatives Assessment Criteria for Hazard Evaluation"⁴ and the GreenScreen for Safer Chemicals v1.2 methods⁵. Any differences in interpretation are explained and justified in this GreenScreen report.

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Licensed Profiler or Certified Practitioner (specify): N/A	

Confirm application of the *Disclosure and Assessment Rules and Best Practice*⁶: (List any deviations)

Disclosure thresholds applied by DfE are unclear in the DfE report.

¹ Use GreenScreen® Assessment Procedure (Guidance) V1.2

² "NON-VERIFIED" means that Verification Has Not Been Performed on this GreenScreen Assessment

³ An Alternatives Assessment for the Flame Retardant Decabromodiphenylether (DecaBDE) Final Report Available at: <u>http://www.epa.gov/dfe/pubs/projects/decaBDE/deca-report-complete.pdf</u>, accessed 2/9/2014

⁴ Available at: <u>http://www.epa.gov/dfe/alternatives_assessment_criteria_for_hazard_eval.pdf</u>, accessed 10/2013.

⁵ Details available at: <u>http://www.cleanproduction.org/Greenscreen.v1-2.php</u>, accessed 10/2013.

⁶ See GreenScreen Guidance V1.2 Section 8

Chemical Name (CAS #):

N-alkoxy Hindered Amine Reaction Products (CAS#191680-81-6)

Also Called:

1,3-Propanediamine, N1,N1'-1,2-ethanediylbis-, reaction products with cyclohexane and peroxidized N-butyl-2,2,6,6-tetramethyl-4-piperidinamine-2,4,6-trichloro-1,3,5-triazine reaction products (TSCA Inventory)

Tradenames:

Flamestab Nor 116

Suitable analogs or moieties of chemicals used in this assessment (CAS #'s): No analog

Chemical Structure(s):

*Note: Include chemical structure(s) of all suitable analogs (and /or moieties) used in the assessment.



Notes related to production specific attributes⁷:

For Inorganic Chemicals and relevant particulate organics (*if not relevant, list NA*) Define Properties:

- 1. Particle size (e.g., silica of respirable size)
- 2. Structure (e.g., amorphous vs. crystalline)
- 3. Mobility (e.g., water solubility, volatility)
- 4. Bioavailability: As a neat material, N-alkoxy hindered amine reaction products are estimated to not be absorbed by any route of exposure. This compound is expected to have poor absorption through all routes when in solution. This material is predominately a polymer with a molecular weight (MW) >1,000 however at present there is no MW cutoff for the hindered amine category of new chemicals.

For Polymeric Materials: (*delete this section if not a polymeric material*) Identify Monomers and Corresponding Properties

According to the DfE report, "This alternative is a polymer. The structure shown is the simplest depiction of an oligomer with a MW <1,000 (approximately 770) that includes all combinations of monomers. This review assesses oligomers with a MW <1,000 using a representative structure. The

⁷ Note any composition or hazard attributes of the chemical product relevant to how it is manufactured. For example, certain synthetic pathways or processes result in typical contaminants, by-products or transformation products. Explain any differences between the manufactured chemical product and the GreenScreen assessment of the generic chemical by CAS #.

representative structure lies within the domain of the available estimation methods. EPI v4.0 estimation methods were used for physical/chemical and environmental fate values in the absence of experimental data. The higher MW oligomers with a MW >1,000 are assessed together using the SF polymer assessment criteria (Boethling et al., 1997)."

"The MF and MW of this polymer are variable; approximately 90% of the oligomers in this polymer have a MW >1,300 (NICNAS, 2001). The mixture is based on a substituted aliphatic tetra amine, where the substituents on the amine groups are variable. The presence of material in the commercial product with a MW <670 is likely the result of unchanged starting materials."⁸

Further information on the following was not available in the DfE report.

- 1. % of Each Monomer
 - a) Monomer 1
 - b) Monomer 2
 - c) Monomer 3
- 2. Are the monomers blocked? (Y/N)
- 3. Molecular Weight (MW) of polymeric material
- 4. % of polymeric material with
 - a) MW <500
 - b) MW <1,000 90% of the oligomers in this polymer have a MW >1,300
- 5. % Weight Residual Monomers
- 6. Solubility/Dispersability/Swellability
- 7. Particle size
- 8. Overall charge of polymeric material
- 9. Identify constituents and residual concentrations of
 - a) Catalysts
 - b) Processing aids
- 10. Identify any monomers, oligomers, catalysts or processing aids classified as Benchmark 1 according to the hazard identification lists in the GreenScreen List Translator.

Identify Applications/Functional Uses:

(e.g., Cleaning product, TV casing)

1. Flame Retardant

GreenScreen Benchmark Score and Hazard Summary Table:^{9,10,11,12}

N-alkoxy hindered amine reaction products was assigned a <u>Benchmark Score of 1</u> based on high group I human toxicity endpoints (reproductive toxicity and developmental toxicity); high group II toxicity endpoints (repeat dose systemic toxicity) and very high aquatic toxicity (acute and chronic) along with very high persistence.

⁸ An Alternatives Assessment for the Flame Retardant Decabromodiphenylether (DecaBDE) Final Report Available at: <u>http://www.epa.gov/dfe/pubs/projects/decaBDE/deca-report-complete.pdf</u>, p 4-468.

⁹ See Appendix A for a glossary of hazard endpoint acronyms

¹⁰ See Appendix B for alternative GreenScreen Hazard Summary Table (Classification presented by exposure route)

¹¹ For inorganic chemicals only, see GreenScreen Guidance V1.2 Section 14.4. (Exceptions for Persistence)

¹² For Systemic Toxicity and Neurotoxicity, repeated exposure data are preferred. Lack of single exposure data is not a Data Gap when repeated exposure data are available. In that case, lack of single exposure data may be represented as NA instead of DG. See GreenScreen Guidance V1.2 Section 9.3.

Green Screen Hazard Ratings: [N-alkoxy hindered amine reaction products]																			
Group I Human					Group II and II* Human							Ecotox		Fate		Physical			
С	Μ	R	D	Е	AT		ST	Ν		SnS*	SnR*	IrS	IrE	AA	CA	Р	B	Rx	F
						single	repeated*	single	repeated*										
М	L	Η	Η	DG	L		Н		L	L	DG	L	М	vH	vH	vH	Η	L	L

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect estimated values, authoritative B lists, screening lists, weak analogues, and lower confidence. Hazard levels in **BOLD** font are used with good quality data, authoritative A lists, or strong analogues. Group II Human Health endpoints differ from Group II* Human Health endpoints in that they have four hazard scores (i.e., vH, H, M and L) instead of three (i.e., H, M and L), and are based on single exposures instead of repeated exposures.

Environmental Transformation Products and Ratings¹³: Identify feasible and relevant environmental transformation products (i.e., dissociation products, transformation products, valence states) and/or moieties of concern¹⁴

Functional Use	Life Cycle Stage	Transformation Pathway	Environmental Transformation Products	CAS #	Feasible and Relevant?	GreenScreen List Translator Score or GreenScreen Benchmark Score
			None			

Introduction

Hazard Classification Summary Section:

For all hazard endpoints:

- Search all GreenScreen specified lists. Report relevant results either in each hazard endpoint section or attach to the end of the report.
- Always indicate if suitable analogs or models were used.
- Attach modeling results (See Appendix C).
- Include all references either in each hazard endpoint section or at the end of the report.

Group I Human Health Effects (Group I Human)

Carcinogenicity (C) Score (H, M or L): M

N-alkoxy Hindered Amine Reaction Products was assigned a score of MODERATE for Carcinogenicity based on a moderate score within the EPA's DfE alternatives assessment. The moderate designation in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. No insight was provided into how the moderate sore was concluded and is therefore is reported in italics within the GreenScreen assessment.

¹³ See GreenScreen Guidance V1.2 Section 13

¹⁴ A moiety is a discrete chemical entity that is a constituent part or component of a substance. A moiety of concern is often the parent substance itself for organic compounds. For inorganic compounds, the moiety of concern is typically a dissociated component of the substance or a transformation product.

The summary provided within the EPA's alternatives assessment was as follows: MODERATE: There is uncertainty due to lack of data for this substance. EPA does not expect this substance to be carcinogenic; however such effects cannot be ruled out.

Mutagenicity/Genotoxicity (M) Score (H, M or L): L

N-alkoxy hindered amine reaction products was assigned a score of LOW for Mutagenicity based on a low score within the EPA's DfE alternatives assessment. The low designation in both GreenScreen and EPA's Alternatives assessment is based on the same measured endpoints. The score was based on *in vitro* test data for exposures to N-alkoxy hindered amine reaction products with no *in vivo* data and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows: LOW: N-alkoxy hindered amine reaction products did not induce gene mutations in Salmonella typhimurium or Escherichia coli and did not induce chromosomal aberrations in Chinese hamster ovary (CHO) cells in the presence and absence of metabolic activation.

Reproductive Toxicity (R) Score (H, M, or L): *H*

N-alkoxy hindered amine reaction products was assigned a score of HIGH for Reproductive Toxicity based on a high score within the EPA's DfE alternatives assessment. For reproductive toxicity EPA's DfE uses numerical data quantifying the hazard associated with the 3 different hazard levels, whereas Green-Screen does not base the hazard score on a numerical rating system but bases classifications on listing under GHS, the EU, and NTP. Therefore conversion of DfE's developmental and reproductive toxicity conclusions to comparable GreenScreen hazard scores is done on a case by case basis. DfE's high score was estimated based on analogy to hindered amines similar in structure. The score was based on professional judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows: HIGH: Estimated potential for reproductive effects based on analogy to other hindered amines similar in structure.

Developmental Toxicity incl. Developmental Neurotoxicity (D) Score (H, M or L): H

N-alkoxy hindered amine reaction products was assigned a score of HIGH for Developmental Toxicity based on a high score within the EPA's DfE alternatives assessment. For developmental toxicity EPA's DfE uses numerical data quantifying the hazard associated with the 3 different hazard levels, whereas Green-Screen does not base the hazard score on a numerical rating system but bases classifications on listing under GHS, the EU, and NTP. Therefore the conversion of DfE's developmental and reproductive toxicity conclusions to comparable GreenScreen hazard scores is done on a case by case basis. DfE's high score was estimated based on analogy to hindered amines similar in structure. The score was based on professional judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows: HIGH: Estimated potential for developmental effects based on analogy to other hindered amines similar in structure.

Endocrine Activity (E) Score (H, M or L): DG

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N-alkoxy hindered amine reaction products was assigned a score of DATA GAP for Endocrine Activity based on no data located.

The summary provided within the EPA's alternatives assessment was as follows: No data located.

Group II and II* Human Health Effects (Group II and II* Human)

Note: Group II and Group II* endpoints are distinguished in the v 1.2 Benchmark system (the asterisk indicates repeated exposure). For Systemic Toxicity and Neurotoxicity, Group II and II* are considered sub-endpoints. When classifying hazard for Systemic Toxicity/Organ Effects and Neurotoxicity endpoints, repeated exposure results are required and preferred. Lacking repeated exposure results in a data gap. Lacking single exposure data does not result in a data gap when repeated exposure data are present (shade out the cell in the hazard table and make a note). If data are available for both single and repeated exposures, then the more conservative value is used.

Acute Mammalian Toxicity (AT) Group II Score (vH, H, M or L):): L

N-alkoxy hindered amine reaction products were assigned a score of LOW for Acute Mammalian Toxicity. The acute mammalian toxicity classification in both the EPA's DfE and GreenScreen is based on the same measured endpoints. The acute mammalian toxicity score was based on test data and therefore is not reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows: LOW: Based on an acute oral $LD_{50} >5,000 \text{ mg/kg}$ and an acute dermal $LD_{50} >2,000 \text{ mg/kg}$ for rats.

Systemic Toxicity/Organ Effects incl. Immunotoxicity (ST)

(ST-single) Group II Score (single dose: vH, H, M or L):

DfE evaluates Systemic Toxicity based on repeated exposures. Lack of data for Systemic Toxicity based on a single exposure does not constitute a data gap when data for repeated exposures are available.

(ST-repeat) Group II* Score (repeated dose: H, M, L): H

N-alkoxy hindered amine reaction products was assigned a score of HIGH for Systemic Toxicity/Organ Effects based on a high score reported within the DfE report. The DfE score is estimated based on analogy hindered amines similar in structure and associated with toxicity to liver, blood and gastrointestinal tract. The high score was based the use of analogs even though experimental data reported that N-alkoxy hindered amine reaction products did not produce adverse effects in a 28-day oral gavage study in rats at oral doses up to 1,000 mg/kg/day. In addition the DfE report indicates the potential exists for immunotoxic effects based on analogy to other hindered amines similar in structure. Therefore the GreenScreen high score is reported in italics.

The summary provided within the EPA's alternatives assessment was as follows: HIGH: Estimated potential for repeated dose effects based on analogy to other hindered amines similar in structure. Experimental data reported N-alkoxy hindered amine reaction products did not produce adverse effects in a 28-day oral gavage study in rats at oral doses up to 1,000 mg/kg/day; however uncertainty remains for exposure of longer duration.

In addition, there is an estimated potential for immunotoxic effects based on analogy to other hindered amines similar in structure.

Neurotoxicity (N)

(N-single) Group II Score (single dose: vH, H, M or L):

DfE evaluates Neurotoxicity based on repeated exposures. Lack of data for Neurotoxicity based on a single exposure does not constitute a data gap when data for repeated exposures are available.

(N-repeat) Group II* Score (repeated dose: H, M, L): L

N-alkoxy hindered amine reaction products was assigned a score of LOW for Neurotoxicity based on a low score within the EPA's DfE alternatives assessment. This conclusion within the DfE report was based on expert judgment with no additional information provided. The low designation in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on expert judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows: LOW: Estimated not to have potential for neurotoxicity based on expert judgment. No data located.

Skin Sensitization (SnS) Group II* Score (H, M or L): L

N-alkoxy hindered amine reaction products were assigned a score of LOW for Skin Sensitization. The low designation for skin sensitization in both GreenScreen and EPA's alternatives assessment is based on the same measured endpoints. The score was based on test data within EPA's alternatives assessment and therefore is not reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows: LOW: N-alkoxy hindered amine reaction products did not produce skin sensitization in an experimental study in guinea pigs.

Respiratory Sensitization (SnR) Group II* Score (H, M or L): DG

N-alkoxy hindered amine reaction products were assigned a score of DATA GAP for Respiratory sensitization. This conclusion was made based on no data located.

Skin Irritation/Corrosivity (IrS) Group II Score (vH, H, M or L): L

N-alkoxy hindered amine reaction products was assigned a score of LOW for Skin Irritation/Corrosivity based on tests results provided within the EPA's DfE alternatives assessment which indicates it is not irritating to rabbit skin. DfE categorizes N-alkoxy hindered amine reaction products as a very low dermal irritant which corresponds to a low score under GreenScreen Skin Irritation/Corrosivity. The score was based on a report from a reliable secondary source within EPA's alternatives assessment and therefore is not reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows: VERY LOW: N-alkoxy hindered amine reaction products are not irritating to rabbit skin.

Eye Irritation/Corrosivity (IrE) Group II Score (vH, H, M or L): M

N-alkoxy hindered amine reaction products was assigned a score of MODERATE for Eye Irritation based on tests results provided within the EPA's DfE alternatives assessment. DfE categorizes N-alkoxy hindered amine reaction products as a low eye irritant which corresponds to a moderate score under GreenScreen Eye Irritation/Corrosivity. The score was based on test data within EPA's alternatives assessment and therefore is not reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

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LOW: N-alkoxy hindered amine reaction products, was slightly irritating to rabbit eyes with clearing within 24 hours.

Ecotoxicity (Ecotox)

Acute Aquatic Toxicity (AA) Score (vH, H, M or L): vH

N-alkoxy hindered amine reaction products were assigned a score of VERY HIGH for Acute Aquatic Toxicity. While the DfE report indicates a high hazard for N-alkoxy hindered amine reaction products, information provided within the alternatives assessment indicated that estimated $L(E)C_{50}$ values are less than 1 mg/L which corresponds to a very high hazard score in GreenScreen. The score was based on professional judgment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows: HIGH: Based on estimated acute aquatic toxicity values for fish, daphnid and green algae using polycationic polymer SAR.

Chronic Aquatic Toxicity (CA) Score (vH, H, M or L): vH

N-alkoxy hindered amine reaction products were assigned a score of VERY HIGH for Chronic Aquatic Toxicity. While the DfE report indicates a high hazard for N-alkoxy hindered amine reaction products, information provided within the alternatives assessment indicated that estimated $L(E)C_{50}$ values are less than 0.1 mg/L which corresponds to a very high hazard score in GreenScreen. The score was based on professional judgment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows: HIGH: Based on estimated chronic aquatic toxicity values for fish, daphnid and green algae using polycationic polymer SARs.

Environmental Fate (Fate)

Persistence (P) Score (vH, H, M, L, or vL): vH

N-alkoxy hindered amine reaction products were assigned a score of VERY HIGH for Persistence. While the DfE reports a high score for persistence, professional judgment included in the alternatives assessment indicates the N-alkoxy hindered amine reaction products will be recalcitrant in the environment and has an estimated environmental half-life in the atmosphere of >180 days. The score was based on expert judgment within EPA's alternatives assessment and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

HIGH: The persistence for N-alkoxy hindered amine reaction products is based on an experimental guideline biodegradation study (4% removal after 28 days). Approximately 90% of the commercial N-alkoxy hindered amine reaction products substance has a MW >1,300 and is not anticipated to be assimilated by microorganisms. This polymer is not expected to be removed by other degradative processes under environmental conditions, such as hydrolysis, since it lacks the functional groups that hydrolyze under environmental conditions. This polymer does not contain chromophores that absorb at wavelengths >290 nm and therefore is not expected to be susceptible to direct photolysis by sunlight. The atmospheric half-life is estimated to be 19 minutes, although it is expected to exist primarily in the particulate phase in air.

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Bioaccumulation (B) Score (vH, H, M, L, or vL): H

N-alkoxy hindered amine reaction products were assigned a score of HIGH for Bioaccumulation. The high designation for bioaccumulation in EPA's alternatives assessment and GreenScreen is based on the same measured endpoints. The DfE score was based on an estimated BAF value and therefore is reported in italics within the GreenScreen assessment.

The summary provided within the EPA's alternatives assessment was as follows:

HIGH: A representative oligomer (with MW 770) that includes all combinations of monomers has an estimated BAF of 2,300; this BAF value, which accounts for metabolism, suggests that this substance has potential to bioaccumulate in higher trophic levels.

Physical Hazards (Physical)

Reactivity (Rx) Score (vH, H, M or L): *L*

N-alkoxy hindered amine reaction products were assigned a score of LOW for Reactivity. EPA does not assess reactivity as one of its hazard criteria and, therefore, no data was available in the EPA assessment to address this criterion. However, professional evaluation of N-alkoxy hindered amine reaction products suggests it is neither reactive nor explosive. Based upon this professional judgment, the reviewer believes a score of 'low' is appropriate.

Flammability (F) Score (vH, H, M or L): L

N-alkoxy hindered amine reaction products was assigned a score of LOW for Flammability based on a not flammable description within the DfE report. This conclusion was based on adequate data and is not reported in italics.

References (may be provided under each hazard endpoint or at the end of document)

APPENDIX A: Hazard Benchmark Acronyms (alphabetical order)

- (AA) Acute Aquatic Toxicity
- (AT) Acute Mammalian Toxicity
- **(B)** Bioaccumulation
- (C) Carcinogenicity
- (CA) Chronic Aquatic Toxicity
- (Cr) Corrosion/ Irritation (Skin/ Eye)
- **(D)** Developmental Toxicity
- (E) Endocrine Activity
- (F) Flammability
- (IrE) Eye Irritation/Corrosivity
- (IrS) Skin Irritation/Corrosivity
- (M) Mutagenicity and Genotoxicity
- (N) Neurotoxicity
- (P) Persistence
- (R) Reproductive Toxicity
- (Rx) Reactivity
- (SnS) Sensitization-Skin
- (SnR) Sensitization-Respiratory
- (ST) Systemic/Organ Toxicity